Crystal monochromators make use of the periodicity of 'perfect' crystals to select the desired photon energy from a range of photon energies. This is described by Bragg's law,

$$2d_{hkl} \sin\theta = n\lambda, \qquad (4.2.5.5)$$

where d_{hkl} is the spacing between the planes having Miller indices hkl, θ is the angle of incidence, n is the order of a particular reflection ($n = 1, 2, 3, \ldots$), and λ is the wavelength.

If there are wavelength components with values near $\lambda/2$, $\lambda/3$, ..., these will be reflected as well as the wanted radiation, and harmonic contamination can result. This can be a difficulty in spectroscopic experiments, particularly XAFS, XANES and DAFS (Section 4.2.3).

Equation (4.2.5.5) neglects the effect of the refractive index of the material. This is usually omitted from Bragg's law, since it is of the order of 10^{-5} in magnitude. Because the refractive index is a strong function of wavelength, the angles at which the successive harmonics are reflected are slightly different from the Bragg angle of the fundamental. This fact can be used in multiple-reflection monochromators to minimize harmonic contamination.

As can be seen in Fig. 4.2.5.4, each Bragg reflection has a finite line width, the Darwin width, arising from the interaction of the radiation with the periodic electron charge distribution. [See, for example, Warren (1968) and Subsection 7.2.2.1.] Each Bragg reflection therefore contains a spread of photon energies. The higher the Miller indices, the narrower the Darwin width becomes. Thus, for experiments involving the Mössbauer effect, extreme back-reflection geometry is used at the expense of photon flux.

If the beam propagates through the specimen, the geometry is referred to as *transmission*, or *Laue*, geometry. If the beam is reflected from the surface, the geometry is referred to as *reflection*, or *Bragg*, geometry. Bragg geometry is the most commonly used in the construction of crystal monochromators. Laue geometry has been used in only a relatively few applications until recently. The need to handle high photon fluxes with their associated high power load has led to the use of diamond crystals in Laue configurations as one of the first components of X-ray optical systems (Freund, 1993). Phase plates can be created using the Laue geometry (Giles *et al.*, 1994). A schematic diagram of a system used at the European Synchrotron Radiation Facility is shown in Fig. 4.2.5.5. Radiation from an insertion device falls on a Laue-geometry pre-monochromator and then passes through a channel-cut (multiple-reflection) monochromator. The strong linear polarization from the source and the monochromators can be changed into circular polarization by the asymmetric Laue-geometry polarizer and analysed by a similar Laue-geometry analysing crystal.

More will be said about polarization in §4.2.5.4.4 and Section 6.2.2.

4.2.5.4.2. *Laboratory monochromator systems*

Many laboratories use powder diffractometers using the Bragg–Brentano configuration. For these, a sufficient degree of monochromatization is achieved through the use of a diffracted-beam monochromator consisting of a curved-graphite monochromator and a detector, both mounted on the 2θ arm of the diffractometer. Such a device rejects the unwanted $K\beta$ radiation and fluorescence from the sample with little change in the magnitude of the $K\alpha$ lines. Incident-beam monochromators are also used to produce closely monochromatic beams of the desired energy. Single-reflection monochromators used for the reduction of spectral energy spread are described in Subsections 2.2.7.2 and 2.3.5.4.

For most applications, this simple means of monochromatization is adequate. Increasingly, however, more versatility and accuracy are being demanded of laboratory diffractometer systems. Increased angular accuracy in both the θ and 2θ axes, excellent monochromatization, and parallel-beam geometry are all demands of a user community using improved techniques of data collection and data analysis. The necessity to study thin films has generated a need for accurately collimated beams of small cross section, and there is a need to have well collimated and monchromatic beams for the study of rough surfaces. This, coupled with the need to analyse data using the Rietveld method (Young, 1993), has caused a revolution in the design of commercial diffractometers, with the use of principles long since used in synchrotron-radiation research for the design of laboratory instruments. Monochromators of this type are briefly discussed in §4.2.5.4.3.

4.2.5.4.3. *Multiple-reflection monochromators for use with laboratory and synchrotron-radiation sources*

Single-reflection devices produce reflected beams with quite wide, quasi-Lorentzian, tails (Subsection 2.3.3.8), a situation

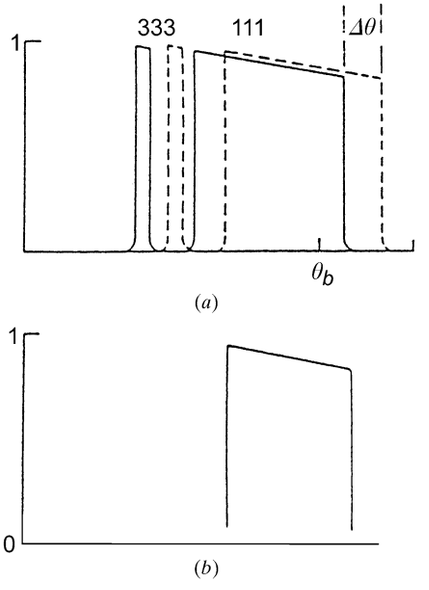

Fig. 4.2.5.4. In (*a*), the schematic rocking curve for a silicon crystal in the neighbourhood of the 111 Bragg peak is shown. The full curve is due to the crystal set to the true Bragg angle, and the dotted curve corresponds to a surface tilted at an angle of 2″ with respect to the beam prior to the acquisition of the rocking curve. Only the 111 and 333 reflections are shown for clarity. The 222 reflection is very weak because the geometrical structure factor is small. The separation of the 111 and 333 peaks occurs because the refractive index is different for these reflections. In a double-crystal monochromator, white radiation from the source will produce the scattered intensity given by the full curve. If that intensity distribution now falls on the second crystal, which is tilted with respect to the first, an angle of tilt can be found for which the Bragg condition is not fulfilled in the second crystal, and the 333 radiation cannot be reflected. The resultant reflected intensity is shown in (*b*). Note that this is an idealized case, and in practice the existence of tails in the reflectivity curve can allow the transmission of some harmonic radiation through the double-crystal monochromator.

references